

# Theory of the Fermi Arcs, the Pseudogap, $T_c$ and the Anisotropy in k-space of Cuprate Superconductors

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The appearance of the Fermi arcs or gapless regions at the nodes of the Fermi surface just above the critical temperature is described through self-consistent calculations in an electronic disordered medium. We develop a model for cuprate superconductors based on an array of Josephson junctions formed by grains of inhomogeneous electronic density derived from a phase separation transition. This approach provides physical insights to the most important properties of these materials like the pseudogap phase as forming by the onset of local (intragrain) superconducting amplitudes and the zero resistivity critical temperature  $T_c$  due to phase coherence activated by Josephson coupling. The formation of the Fermi arcs and the dichotomy in k-space follows from the direction dependence of the junctions tunneling current on the d-wave symmetry on the  $CuO_2$  planes. We show that this semi-phenomenological approach reproduces also the main features of the cuprates phase diagram.

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A convincing explanation to the origin of the pseudogap and the dome-like shape of the superconducting critical temperature  $T_c(p)$  on the doping level  $p$  of the copper oxide superconductors has become a major long standing challenge in condensed matter physics. The lack of a well accepted theory is likely to be due to the nanoscale complexity and the intrinsically inhomogeneous electronic structures[1, 2] that are not easy to be mathematically characterized. Recently, new techniques were developed to control the level of phase separation of dopant oxygen interstitials in  $La_2CuO_{4+y}$  and established a direct correspondence between the degree of order and the values of  $T_c$ [3, 4] paving the way to new theoretical treatments.

Electronic inhomogeneities in cuprates were verified by several different experiments: neutron diffraction[5–7], muon spin relaxation ( $\mu SR$ )[8, 9], nuclear quadrupole resonance (NQR) and nuclear magnetic resonance (NMR)[10, 11] have detected some form of disordered local electronic densities. The nanometer spatial variations of the electronic gap amplitude  $\Delta(\vec{r})$  measured by atomically resolved spectroscopy such as scanning tunneling microscopy (STM)[12–15] is possibly related with the charge inhomogeneities. Angle resolved photon emission spectroscopy (ARPES) found a large anisotropy in k-space: a larger gap at the leading edge of the Fermi surface or antinodal (along the  $Cu - O$  bonds) direction  $((\pm\pi, 0)$  and  $(0, \pm\pi))$ [16] that remains well above  $T_c$  and a small d-wave like gap that vanishes at the nodal direction.

More recently, ARPES experiments measured nodal gapless Fermi arcs starting at  $T_c$  and increasing with the temperature while the antinodal gaps remained almost constants[17]. Another group revealed a metallic dispersion along the Fermi arcs and a Bogoliubov-like dispersion toward the antinodal regions either above and below  $T_c$ [18] demonstrating the presence of the superconducting amplitudes above  $T_c$ . Electronic Raman

scattering experiments[19] showed that the nodal gap is connected with  $T_c$  and the antinodal with the pseudogap. Intrinsic tunneling spectroscopy also measured a gap that closes at  $T_c$  and a pseudogap that virtually does not change with the temperature and remains above  $T_c$ [20], in agreement with two energy scales in cuprate superconductors[17, 19].

To describe these complex phenomena some theories producing phase separation have been suggested, mainly based on doped Mott-Hubbard insulators[21–25]. While they describe some of the observed features, they fail to predict all the details related with real space inhomogeneities and the k-space dichotomy. While these theories describe some of the observed features of cuprates, they fail, for instance, to predict all the details related with real space inhomogeneities and the k-space dichotomy. To deal with this problems some theories considered the presence of impurities or inhomogeneities in the local electronic distribution as a starting point to derive the superconducting properties[26, 27]. Some others approaches used the influence of a mesoscopic phase separation in the appearance of superconductivity to derive the general properties of cuprates[28, 29].

In this letter we show that it is possible to find an unified explanation to all these experiments starting with an electronic phase separation EPS forming small granular regions where isolated superconducting amplitudes may be formed. The origin of the EPS may be due to the lower free energy of the low density anti-ferromagnetic domains[30]. These local d-wave superconducting amplitudes in these islands form an array of multiple Josephson junctions[31, 32]. In a typical d-wave superconductors junction the direction dependence of the tunnel matrix elements that describe the barrier is relevant[33]. In the case of cuprates, all the domains have d-wave pair wave functions with the same direction with respect to the  $a$  and  $b$  crystal axis. Phase fluctuation above  $T_c$  generates

the gapless region that increases with temperatures at the nodal direction where the d-wave superconducting gap is smaller and accounts for the k-space anisotropy.

To describe mathematically the electronic phase separation of high  $T_c$  oxides we use the time dependent Cahn-Hilliard (CH) equation[34]. In this approach it is possible to follow the formation of domains with distinct local densities below the phase separation transition temperature  $T_{PS}$ .  $T_{PS} = T_{PS}(p)$  is likely to be close the upper pseudogap temperature since  $T_{PS}(p)$  may be the cause of some observed high temperature anomalies[35]. The time  $t$  in the CH equation is related with the temperature  $T$ ; larger times correspond to lower temperatures below  $T_{PS}(p)$  and consequently, larger disorder[29, 30, 36, 37]. In the disordered phase the appropriate order parameter is the difference between the local and the average charge density  $p$ ,  $u(p, i, T) \equiv (p(i, T) - p)/p$ .  $u(i, T) = 0$  corresponds to the homogeneous case above  $T_{PS}(p)$  and the Ginzburg-Landau (GL) free energy functional is given by the usual power expansion,

$$f(u) = \frac{1}{2}\varepsilon^2|\nabla u|^2 + V_{GL}(u, T). \quad (1)$$

Where the potential  $V_{GL}(u, T) = -A^2(T)u^2/2 + B^2u^4/4 + \dots$ ,  $A^2(T)/B = \alpha(T_{PS}(p) - T)$  for  $T < T_{PS}$ ,  $\alpha$  is a constant.  $\varepsilon$  gives the size of the barrier between the low and high density phases [29, 36]. The CH equation can be written[38] in the form of a continuity equation of the local density of free energy  $f$ ,  $\partial_t u = -\nabla \cdot \mathbf{J}$ , with the current  $\mathbf{J} = M\nabla(\delta f/\delta u)$ , where  $M$  is the mobility or the charge transport coefficient that sets the phase separation time scale. Therefore,

$$\frac{\partial u}{\partial t} = -M\nabla^2(\varepsilon^2\nabla^2 u - A^2(T)u + B^2u^3). \quad (2)$$

In Fig.(1), we show a typical  $V_{GL}(u, T)$  simulation where the barriers between different grains are clearly visible. We have argued in previous works[31, 32] that the particles may become confined in these domains increasing the probability of Cooper pair formation. In our calculations we take into account that these free energy barriers are essentially constant at low temperatures and varies as  $(T_{ps} - T)^{1.5}$  near the transition as shown by CH[34].

Then, after performing the CH simulations, the local disorder density  $p(i, T)$  is used as the *initial input* and *it is maintained fixed* throughout the self-consistent Bogoliubov-deGennes (BdG) method. This method yields local varying d-wave amplitudes  $\Delta_c(i, p, T)$  as demonstrated previously[30–32, 37].

As mentioned above,  $V_{GL}(p, T)$  favors the charge to be confined into the domains acting as a catalyst to Cooper pair formation. We have showed that the two-body attractive potential of the BdG equation is scaled by the height of the free energy barriers shown in Fig.(3). In Ref.[32] we called it the grain boundary potential  $V_{gb}$ . Here we generalize it to any doping value by

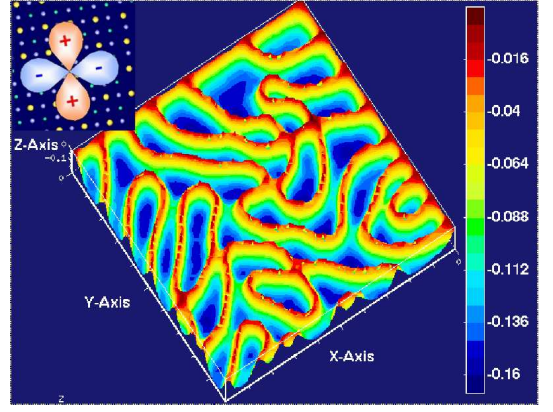


FIG. 1. (color online) Typical solution of the free energy potential  $V_{GL}(u, T)$  on a  $50 \times 50$  lattice. At low temperatures the charges are attracted to the grains, similar to a granular superconductor. On the top left is shown the d-wave superconducting amplitude in these bound regions.

the expression,  $V_{gb}(p) = -14.2 + 45 \times p$  (eV). With this two-body attractive potential a typical BdG solution  $\Delta_d(p = 0.15, i, T)$  is shown in Fig.(2) for five different grains “i”. The low temperature values between 30-70meV are in the energy range of the LDOS gaps measured by STM experiments on Bi2212[12–15].

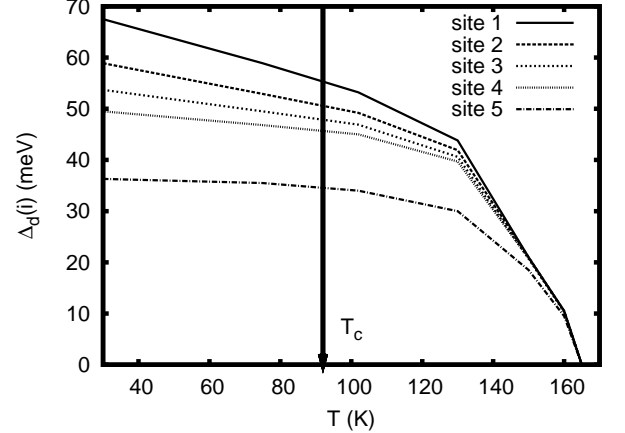


FIG. 2. The temperature evolution of  $\Delta_d(i)$  at five different locations of a  $p = 0.15$  compound. The mean-field BdG calculations all vanishes at the same temperature  $T^*(0.15) \approx 165$ K (above  $T_c(0.15) = 92$ K). The low temperature values between 30-70meV are in the energy range of the Bi2212 LDOS gaps measured by STM.

To obtain the experimental values of  $T_c(p)$ , we use an approach similar to a system composed of granular superconductors[41]. Our main proposal is that the superconducting transition occurs in two steps as  $T$  decreases[31, 32, 37]: first by intra-grain superconductivity and then by Josephson coupling with phase locking at low temperatures.

These two completely different calculations, yielding two different energy scales, are motivated by the two energy scales found in most cuprates mentioned above[16, 19], and also in the two different regimes of the fluctuation magnetoconductivity in a  $YBa_2Cu_3O_7$  single crystal[42]. These systematic measurements detected an effectively two-dimensional (2D) regime far above  $T_c$ , that can be interpreted in our approach by the isolated superconducting grains in the  $CuO$  without phase coherence. Decreasing the temperature towards  $T_c$  a crossover to a three-dimensional (3D) Gaussian regime sets in as the different superconducting regions or grain become connected and increase coherence. Very close to  $T_c$  a critical regime characteristic of a 3D XY universality class is measured which is consistent with a granular superconductors in which each superconducting grain develops its own phase  $\Phi$  that may oscillate but become locked at  $T_c$ , yielding long range order.

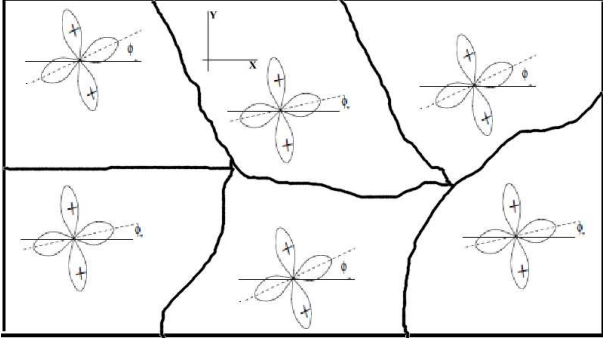


FIG. 3. Schematic figure representing the array of Josephson junctions on a  $CuO_2$  plane. The local dependent amplitudes  $\Delta(p, i, T)$  are represented by the orbitals and the phase angles  $\phi$  oscillates around the crystal  $a$ -axis direction due to the symmetry of the d-wave on the  $CuO_2$  plane.

Consequently, the system is regarded as an array of Josephson junction as shown schematically in Fig.(3). The phenomenology of Josephson tunnel junctions between d-wave superconductors have been developed by Bruder et al[33]. They calculate the tunnel matrix elements in second-order perturbation theory for two superconductors (1 and 2) with superconducting amplitude  $\Delta_{d,1/2}(i, T, \Phi) = \Delta(i, T) \cos[2(\Phi - \phi_{1/2})]$ . We use their results to an array of junction as schematically shown in Fig.(3), where the local amplitudes  $\Delta_d(i, T)$  are represented by the size of orbitals and the phase angles  $\phi$  have been drawn around x-direction.  $\Phi$  is the polar angle of the first Brillouin zone. Due to the thermal energy the gap must be averaged over  $\phi$ , then  $\langle \Delta(p, T, \Phi) \rangle = (\int^{\Delta\phi} \Delta_d^{av}(p, T) \cos[2(\Phi - \phi)] d\phi) / \Delta\phi$ . And  $\Delta_d^{av}(p, T) \equiv \sum_i^N \Delta_d(p, i, T) / N$  is the spatial average superconducting amplitude. At  $T \leq T_c$  the values of  $\phi_{1/2}$  are essentially locked. At  $T \geq T_c$  the phase angles decouple and oscillate within a maximum amplitude that increases with  $T$  as shown in Fig.(3). In this case  $\langle \Delta_d^{av}(p, T) \cos[2(\Phi - \phi)] \rangle$  vanishes when

$2(\Phi - \phi) \approx \pm\pi/4$  or it is less than  $K_B T$ . The results are shown in Fig.(4) and compare well with the  $\Phi$  dependent ARPES measurements of Lee et al[17]. The ap-

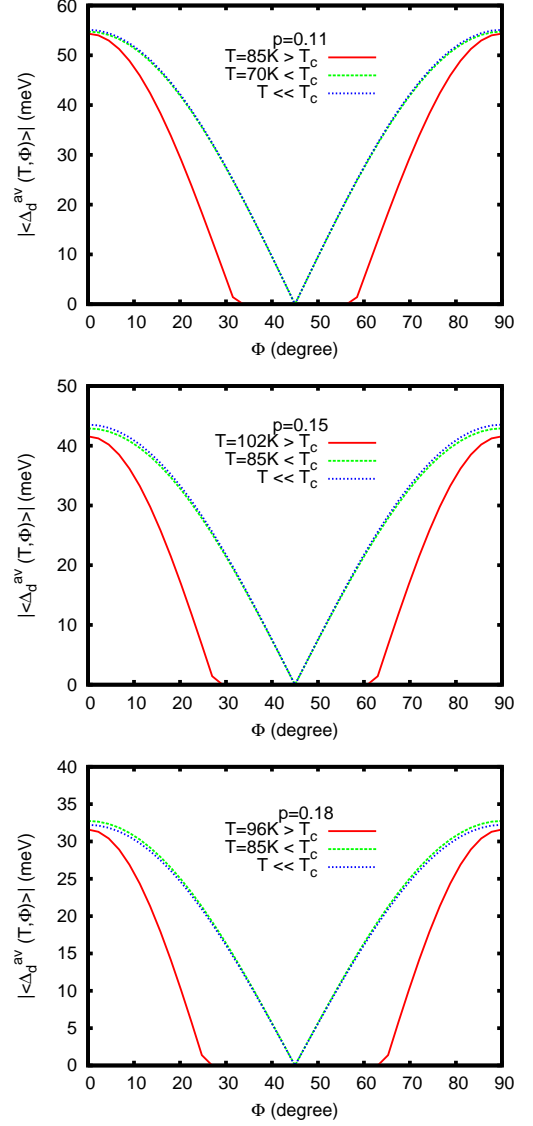


FIG. 4. The absolute value of the spatial and  $\phi$  average,  $\langle \Delta_d^{av}(T, \Phi) \rangle$ , as function of the k-space polar angle  $\Phi$ . The developing of the Fermi arcs around the nodal direction above  $T_c$  is a consequence of the lack of phase coherence and, as measured by ARPES[17, 18],  $\langle \Delta_d^{av}(T, \Phi) \rangle \leq K_B T$ .

pearance of a gapless region around the nodal direction ( $\Phi = \pm\pi/4$ ) above  $T_c$  while the antinodal ( $\Phi = \pm n\pi/2$ ,  $n=1,2,\dots$ ) gap remains almost constant is concordant with the data of Kanigel et al[18]. They found that the electronic dispersion is either metallic along the Fermi arcs or exhibits Bogoliubov-like behavior near the nodes at temperatures above  $T_c$ . This behavior can be understood with the results for  $\Delta_d(i, p, T) \times T$  shown in Fig.(2) and  $\Delta_d^{av}(p, T) \times \Phi$  of Fig.(4).

To calculate the Josephson coupling energy that is connected with the onset of phase coherence, we recall the work of Bruder et al[33]. They found that the tunneling current behaves in a similar fashion of s-wave superconductors junction and the leading behavior is determined by tunneling from a gap node in one side of a junction into the effective gap in the other side. Consequently, as a first approximation to the Josephson coupling energy  $E_J$ , we adapt the theory of s-wave granular superconductors[43] to the  $\Delta_d^{av}(p, T)$  in the grains.

$$E_J(p, T) = \frac{\pi \hbar \Delta_d^{av}(p, T)}{4e^2 R_n(p)} \tanh\left(\frac{\Delta_d^{av}(p, T)}{2K_B T}\right). \quad (3)$$

Where  $R_n(p)$  is the normal resistance of the compound. We use here values proportional to the planar resistivity  $\rho_{ab}$  measured on the  $La_{2-p}Sr_pCuO_2$  series[44] and the estimated values of  $R_n(p)e^2/h$  are plotted in Fig.(5). Since the onset of phase coherence occurs when the thermal energy equals the Josephson coupling,  $K_B T(p) = E_J(p, T)$ , we obtain one of our most important result; the derivation of the dome-like shape dependence of  $T_c(p) = E_J(p, T_c)/K_B$ , as plotted in Fig.(5).

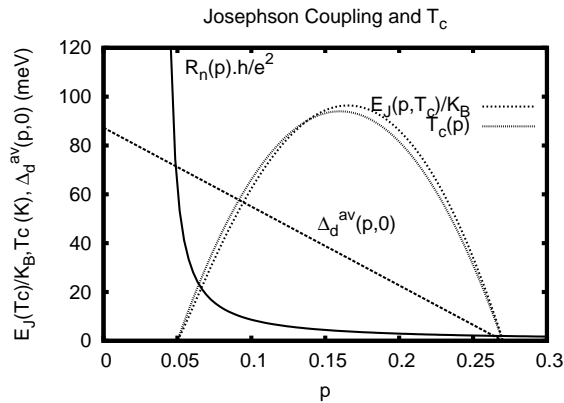


FIG. 5. The temperatures which  $E_J(p, T) = K_B T(p)$  yield  $T_c(p) = E_J(p, T_c)/K_B$ , for comparison we plot also the formula  $T_c(p) = 95(1 - 82.6(p - 0.16)^2)$ . The experimental resistivity  $R_n(p)e^2/h$  used in  $E_J(p, T)$  (Eq.3) is also plotted following Takagi et al[44]. It is also shown the average low temperature gap  $\Delta_d^{av}(p, T = 0)$  that is proportional to the pseudogap temperature  $T^*(p)$ .

To show how  $T_c(p)$  is calculated we plot also in Fig.(5) the average low temperature gap  $\Delta_d^{av}(p, T = 0) \approx \Delta_d^{av}(p, T_c)$  that enters into Eq.(3). As it is shown in Fig.(5), the results agree with empirical formula  $T_c(p) = 95(1 - 82.6(p - 0.16)^2)$ . The dome-like shape is a consequence of the values of  $\Delta_d^{av}(p, T)$  that increases as  $p$  decreases while  $1/R_n(p)$  have opposite behavior, it is essentially zero near  $p = 0.05$  and increases with  $p$  (see  $R_n(p)e^2/h$  plotted in Fig.(5)).

In conclusion, the CH disordered free energy in cuprates forms small electronic domains that induces local Cooper pairs and also an array of Josephson junctions, as in a granular superconductor. This approach reproduces important experimental results and provides novel interpretations: The two energy scales measured by electronic Raman spectroscopy[19], tunneling spectroscopy[20] and ARPES[16, 17] are; one associated with the Josephson coupling energy  $E_J(p)$  that follows  $T_c(p)$  and the other related with the d-wave mean superconducting gap  $\Delta_d^{av}(p, T)$  that increases as the doping decreases.

Concerning the k-space anisotropy, the appearance of the Fermi arcs near the nodal direction is due to the lack of phase rigidity among superconducting domains combined with the small d-wave amplitudes around the nodal directions. In this way the existence of Bogoliubov-like dispersions above  $T_c$ , close to the antinodal directions, have the same cause, namely the anisotropic d-wave geometry of the intragrain superconductivity that is larger around these directions and remains just at  $T^*(p)$ , i.e., above  $T_c(p)$ . Consequently the pseudogap phase is composed of these localized superconducting domains without phase coherence and with a nodal metal structure.

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